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Application of a computer-aided framework for the design of CO₂ capture and utilization processes

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Currently, close to 50 gigatonnes per year of carbon dioxide are emitted to the atmosphere. As carbon dioxide is the dominant greenhouse gas that contributes to sustainability concerns, these emissions need to be targeted for reduction. Carbon dioxide capture and utilization shows promise due to the ability to offset (economically) the cost of carbon capture. However, in order to ensure the sustainability of these processes, methods and tools need to be developed and implemented. To this end, a framework for sustainable process synthesis-design, comprising three stages, (1) synthesis, (2) design, and (3) innovation, has been developed. In order to facilitate the implementation and ensure sustainability, this framework integrates a number of computer-aided methods and tools, that are important for carbon dioxide capture and utilization. Applying this framework helps to address the questions about carbon dioxide capture, storage and utilization on several scales (local as well as global). For example, which higher value chemicals can be produced, what are their current demands, and how much of the carbon dioxide would be utilized?

This framework has been applied to the design and analysis of carbon dioxide capture and utilization processes from coal-fired power plant flue gas to produce various value-added chemical products, including methanol, dimethyl carbonate, dimethyl ether, succinic acid and acetic acid, via conversion. First, the processing route is selected from a network of alternatives. This stage incorporates reaction path synthesis to find different reaction opportunities (currently over 100 reactions have been generated producing commercial chemical products), a database to store the information, and an interface, Super-O, to facilitate the synthesis. In this way, unique opportunities and products are explored. Second, the selected processing route is designed and analyzed by using simulation software and sustainability (economic, environmental and LCA) analysis tools. From this stage, hot spots

and areas for improvement are also generated. Third, the targets for improvement are used to develop novel and more sustainable design alternatives, including the use of process intensification. As a result, it is possible to identify non-trade-off carbon dioxide capture and conversion processes. The production of methanol and dimethyl carbonate have been designed and analyzed to show that conversion processes can be economically competitive and environmentally beneficially (carbon dioxide reducing). This work will present the application of reaction path synthesis combined with superstructure optimization and an appropriate database, to propose sustainable processing routes, with negative netCO₂ emissions, for a class of valuable chemicals.